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The Characteristic Finite Volume Element Method for 1-D Semiconductor Device Simulation*

LONG Xiao-han[1], CHEN Chuan-jun[2]

(1- School of Mathematics and Information, Ludong University, Yantai 264025;

2- Department of Mathematics and Information Science, Yantai University, Yantai 264005)

Abstract: The finite volume element method is combined with the characteristic method to treat the one-dimensional semiconductor device simulation problem. A fully discrete implicit Euler characteristic finite volume element scheme is derived and studied. With different time steps for the electrostatic potential and other unknown quantities, the computational procedure of the new method is constructed. A priori convergence estimate of first-order accuracy in L^2-norm is obtained under suitable assumptions. Numerical experiments demonstrate the validity of the theoretical results and efficiency of the method.

Keywords: semiconductor device; characteristic method; finite volume element method; error estimate

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1 Introduction

We consider the following one-dimensional semiconductor device simulation in $\Omega = [a, b]$:

$$-\frac{\partial^2 \psi}{\partial x^2} = \alpha\big(p - e + N(x)\big), \quad (x,t) \in \Omega \times (0, \bar{T}], \tag{1}$$

$$\frac{\partial e}{\partial t} = \frac{\partial}{\partial x}\Big(D_e(x)\frac{\partial e}{\partial x} - \mu_e e \frac{\partial \psi}{\partial x}\Big) - R(e,p,T), \quad (x,t) \in \Omega \times (0, \bar{T}], \tag{2}$$

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\Big(D_p(x)\frac{\partial p}{\partial x} + \mu_p p \frac{\partial \psi}{\partial x}\Big) - R(e,p,T), \quad (x,t) \in \Omega \times (0, \bar{T}], \tag{3}$$

$$\begin{aligned}\rho(x)\frac{\partial T}{\partial t} - \frac{\partial^2 T}{\partial x^2} = \Big[\Big(D_p(x)\frac{\partial p}{\partial x} + \mu_p(x) p \frac{\partial \psi}{\partial x}\Big) \\ - \Big(D_e(x)\frac{\partial e}{\partial x} - \mu_e(x) e \frac{\partial \psi}{\partial x}\Big)\Big] \cdot \frac{\partial \psi}{\partial x}, \quad (x,t) \in \Omega \times (0, \bar{T}],\end{aligned} \tag{4}$$

where (1) is the electrostatic potential equation, (2) and (3) are the electron and hole concentration equations, respectively, and (4) is the temperature equation. The four equations with initial and boundary conditions make up a closed system. $\alpha = q/\varepsilon$, where q and ε are both positive constants, respectively, representing the electron charge and the dielectric permittivity. $D_s(x)\,(s = e, p)$ is the diffusion coefficient and $\mu_s(x)\,(s = e, p)$ is the mobility. $D_s(x)$

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and $\mu_s(x)$ obey the Einstein relation $D_s(x) = U_T\mu_s(x)$, where U_T is the thermal voltage. $N(x) = N_D(x) - N_A(x)$ is a given function, where $N_D(x)$ is the donor impurity concentration and $N_A(x)$ is the acceptor impurity concentration. $R(e,p,T)$ is a recombination term of the electron and hole concentrations with the influence of temperature. For (1)-(4), we consider the initial value conditions

$$e(x,0) = e_0(x), \quad p(x,0) = p_0(x), \quad T(x,0) = T_0(x), \quad x \in \Omega, \tag{5}$$

and the initial value of ψ can be calculated by (1) and (5). For convenience, we assume that problems (1)-(5) are Ω-periodic[1,2]. For ordinary boundary value problems we can obtain the similar results via dealing with the technique extension or mirror reflection[3].

Since Gummel[4] first proposed sequence iterative computational methods for this kind of problem, there have been many numerical contributions on such problems[3,5,6]. Among the semiconductor mathematical models, the electron concentration equation (2) and the hole concentration equation (3) are always convection-dominated. It means that the convection term is distinctly more important than the diffusion term. If we only use pure standard methods such as the finite element method, the finite difference method or the finite volume element method, it will generate numerical dispersion and nonphysical oscillations unless the mesh is excessively impractical. So Douglas and Russell[7,8] proposed the characteristic method and combined the method with the finite element method or the finite difference method. They analyzed the method under Ω-periodic assumptive condition and solved many physical problems with satisfactory results.

In this paper, with the modified characteristic method, we construct a fully discrete implicit Euler characteristic finite volume element method for the one-dimensional semiconductor device simulation. With different time steps for the electrostatic potential and other unknown quantities, we construct the computational procedure of the method. A priori convergence estimate of first-order accuracy in the L^2-norm is obtained under some suitable assumptions. In the end we give numerical experiments to validate the theoretical results.

2 Characteristic finite volume element scheme

Let us discrete the domain $\Omega = [a,b]$ into J subintervals by the points $a = x_0 < x_1 < x_2 < \cdots < x_i < \cdots < x_J = b$. Let $h_i = x_i - x_{i-1}$, $I_i = [x_{i-1}, x_i]$ and $h = \max_{1\le i\le J}$, $i = 1,2,\cdots,J$. Assume that the partition is quasi-uniform, i.e., there is a positive constant $C_0 > 0$ such that $h_i \ge C_0 h$ for all $i = 1,2,\cdots,J$. This partition is denoted by $T_h = \{I_i\}_{i=1}^J$ and the subinterval I_i is called finite element.

We introduce the dual partition T_h^* with nodes

$$x_{i-1/2} = (x_{i-1} + x_i)/2, \quad 1 \le i \le J.$$

Let

$$I_0^* = [x_0, x_{1/2}], \quad I_i^* = [x_{i-1/2}, x_{i+1/2}], \quad I_J^* = [x_{J-1/2}, x_J], \quad 1 \le i \le J-1.$$

I_i^* is also called control volume. Let

$$\bar{H}^1(\Omega) = \{u(x) \in H^1(\Omega),\ \Omega - \text{periodic}\}, \quad \mathcal{U} = \bar{H}^1(\Omega) \cap H^2(\Omega).$$

Then we introduce the solution space $\mathcal{U}_h \subset \mathcal{U}$ of the piecewise linear functions on the original partition of the domain. The basis function with respect to x_i is[9]

$$\varphi_i(x) = \begin{cases} 1 - h_i^{-1}|x - x_i|, & x_{i-1} \le x \le x_i, \\ 1 - h_{i+1}^{-1}|x - x_i|, & x_i \le x \le x_{i+1}, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, for any $u_h \in \mathcal{U}_h$, we have $u_h = \sum_{i=1}^{J} u_i \varphi_i(x)$, where $u_i = u_h(x_i)$.

We choose the test function space $\mathcal{V}_h$ of piecewise constant functions on the dual partition T_h^*. The characteristic function, defined by

$$\varphi_i^*(x) = \begin{cases} 1, & x_{i-1/2} \le x \le x_{i+1/2}, \\ 0, & \text{otherwise,} \end{cases}$$

forms a basis for the space $\mathcal{V}_h$. For any $v_h \in \mathcal{V}_h$, there is $v_h = \sum_{i=1}^{J} v_i \varphi_i^*(x)$, where $v_i = v_h(x_i)$.

By means of the local basis we can introduce the interpolation operators: $I_h : \mathcal{U} \to \mathcal{U}_h$ and $I_h^* : \mathcal{U} \to \mathcal{V}_h$ such that

$$I_h u = \sum_{i=1}^{J} u(x_i)\varphi_i(x), \quad I_h^* u = \sum_{i=1}^{J} u(x_i)\varphi_i^*(x), \quad u \in \mathcal{U}.$$

Define the bilinear form

$$a(D; u, v) = \begin{cases} \displaystyle\int_a^b D \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} \mathrm{d}x, & (u, v) \in \mathcal{U}_h \times \mathcal{U}_h, \\ \displaystyle -\int_a^b \frac{\partial}{\partial x}\Big(D\frac{\partial}{\partial x}u\Big)v \mathrm{d}x, & (u, v) \in \mathcal{U}_h \times \mathcal{V}_h, \end{cases}$$

and $a(1; u_h, v_h) = a(u_h, v_h)$. To give a fully discredited scheme, we take the time step $\Delta t = \bar{T}/N$, where N is a positive integer and $t^n = n\Delta t$, $n = 0, 1, \cdots, N$. Denote $u_h(t^n) = u_h^n$.

Let $\tau_e(x)$ be the unit vector of $(-\mu_e u, 1)$ and $\tau_p(x)$ be the unit vector of $(\mu_p u, 1)$, respectively. Denote $\phi_s = [1 + \mu_s^2 u^2]^{1/2}$ and $s = e, p$. Then the characteristic derivative is approximated by

$$\frac{\partial}{\partial \tau_e} = \frac{1}{\phi_e}\Big(\frac{\partial}{\partial t} - \mu_e u \frac{\partial}{\partial x}\Big), \quad \frac{\partial}{\partial \tau_p} = \frac{1}{\phi_p}\Big(\frac{\partial}{\partial t} + \mu_p u \frac{\partial}{\partial x}\Big).$$

We use a backward difference quotient for $\frac{\partial e^n}{\partial \tau_e}(x) = \frac{\partial e}{\partial \tau_e}(x, t^n)$ along the characteristics. Specifically, we take

$$\phi_e(x)\frac{\partial e^n}{\partial \tau_e} \doteq \phi_e(x)\frac{e^n(x) - e^{n-1}(x + \mu_e u^n \Delta t)}{[(x - \bar{x})^2 + \Delta t^2]^{1/2}} = \frac{e^n(x) - e^{n-1}(x + \mu_e u^n \Delta t)}{\Delta t}. \tag{6}$$

Since the electric potential on time steps always varies slowly in the semiconductor model, we will use large time steps to compute. However, we use small time steps to compute the electron concentration, the hole concentration and the temperature equations. We introduce

the following notation: Δt—the concentration and temperature time step, $\Delta\bar{t}^0$—the first time step of the electric potential equation, and $\Delta\bar{t}$—the other time step of the electric potential equation. Let

$$j = \Delta\bar{t}/\Delta t, \quad j^0 = \Delta\bar{t}^0/\Delta t, \quad t^n = n\Delta t, \quad t_m = \Delta\bar{t}^0 + (m-1)\Delta\bar{t}.$$

For a function $\psi(x,t)$, let

$$\psi^n = \psi(t^n), \quad \psi_m = \psi(t_m), \quad \partial_t\psi^n = (\psi^{n+1} - \psi^n)/\Delta t,$$

$$\partial_t\psi_m = (\psi_{m+1} - \psi_m)/\Delta\bar{t}\ (m > 0), \quad \partial_t\psi_0 = (\psi_1 - \psi_0)/\Delta\bar{t}^0,$$

and

$$E\psi^n = \begin{cases} \psi_0, & t^n \le t_1, \\ (1 + \dfrac{\vartheta}{j^0})\psi_1 - \dfrac{\vartheta}{j^0}\psi_0, & t_1 < t^n \le t_2, \quad t^n = t_1 + \vartheta\Delta t, \\ (1 + \dfrac{\vartheta}{j})\psi_m - \dfrac{\vartheta}{j}\psi_{m-1}, & t_m < t^n \le t_{m+1}, \quad t^n = t_m + \vartheta\Delta t. \end{cases} \tag{7}$$

The subscript is corresponding to the electric potential time level and the superscript is corresponding to the concentration and temperature time level, respectively. $E\psi^n$, which is made up of the previous two time level values, denotes the extrapolation of ψ at t^n. Let

$$u_h = -\frac{\partial\psi_h}{\partial x}, \quad \bar{x}_e^{n-1} = x + \mu_e E u_h^n \Delta t, \quad \bar{e}_h^{n-1} = e_h(\bar{x}_e^{n-1}),$$

$$\bar{x}_p^{n-1} = x - \mu_p E u_h^n \Delta t, \quad \bar{p}_h^{n-1} = p_h(\bar{x}_p^{n-1}).$$

Then a fully-discrete implicit Euler characteristic FVE scheme for the 1-D semiconductor problem can be defined as to find $\{\psi_{h,m}, e_h^n, p_h^n, T_h^n\} \in \mathcal{U}_h$, for $n = 1, 2, \cdots, N$, such that

$$a(\psi_{h,m}, \chi_h) = \alpha(p_{h,m} - e_{h,m} + N_m, \chi_h), \quad \forall\, \chi_h \in \mathcal{V}_h, \tag{8}$$

$$\Big(\frac{e_h^n - \bar{e}_h^{n-1}}{\Delta t}, \omega_h\Big) + a(D_e; e_h^n, \omega_h) - \Big(\bar{e}_h^{n-1} E u_h^n \frac{\partial\mu_e}{\partial x}, \omega_h\Big)$$
$$- \big(\alpha\mu_e e_h^n (\bar{p}_h^{n-1} - \bar{e}_h^{n-1} + N^n), \omega_h\big) + \big(R(e_h^n, p_h^n, T_h^n), \omega_h\big) = 0, \quad \forall\, \omega_h \in \mathcal{V}_h, \tag{9}$$

$$\Big(\frac{p_h^n - \bar{p}_h^{n-1}}{\Delta t}, \omega_h\Big) + a(D_p; p_h^n, \omega_h) + \Big(\bar{p}_h^{n-1} E u_h^n \frac{\partial\mu_p}{\partial x}, \omega_h\Big)$$
$$+ \big(\alpha\mu_p p_h^n (\bar{p}_h^{n-1} - \bar{e}_h^{n-1} + N^n), \omega_h\big) + \big(R(e_h^n, p_h^n, T_h^n), \omega_h\big) = 0, \quad \forall\, \omega_h \in \mathcal{V}_h, \tag{10}$$

$$\Big(\rho\frac{T_h^n - T_h^{n-1}}{\Delta t}, z_h\Big) + a(T_h^n, z_h) = -\Big(D_p \frac{\partial p_h^n}{\partial x} E u_h^n, z_h\Big) + \big(\mu_p p_h^n (E u_h^n)^2, z_h\big)$$
$$+ \Big(D_e \frac{\partial e_h^n}{\partial x} E u_h^n, z_h\Big) + \big(\mu_e e_h^n (E u_h^n)^2, z_h\big), \quad \forall\, z_h \in \mathcal{V}_h, \tag{11}$$

$$e_h^0(x) = (I_h e_0)(x), \quad p_h^0(x) = (I_h p_0)(x), \quad T_h^0(x) = (I_h T_0)(x), \quad x \in \Omega. \tag{12}$$

The algorithm of the computational procedure is as follows. The initial values of e_h^0, p_h^0, T_h^0 are defined by (12); from (8) we can get $\psi_{h,0}$. Assuming that the solutions of $\{\psi_{h,m-1}, e_h^{n-1},$

p_h^{n-1}, $T_h^{n-1}\}$ are obtained, then we can compute the values of e_h^n, p_h^n and T_h^n by (9), (10) and (11). Repeat j times in this way, we can obtain $\psi_{h,m}$ from (8). The whole computational procedure of this algorithm is as follows. e_h^0, p_h^0, T_h^0, $\psi_{h,0}$; e_h^1, p_h^1, T_h^1, $\cdots$, $e_h^{j_0}$, $p_h^{j_0}$, $T_h^{j_0}$, $\psi_{h,1}$; $e_h^{j_0+1}$, $p_h^{j_0+1}$, $T_h^{j_0+1}$, $\cdots$, $e_h^{j_0+j}$, $p_h^{j_0+j}$, $T_h^{j_0+j}$, $\psi_{h,2}$; $\cdots$

3 Error estimate analysis

Now, we consider error estimates in the L^2-norm for the fully discrete characteristic finite volume element scheme (8)-(12). We will introduce some elliptic projections. Let $\tilde{\psi} = \tilde{\psi}_h \in \mathcal{U}_h$, such that

$$a(\psi - \tilde{\psi}, \chi_h) = 0, \quad \forall\, \chi_h \in \mathcal{V}_h, \tag{13}$$

and let $\tilde{e}$, $\tilde{p}$, $\tilde{T} \in \mathcal{U}_h$, satisfy

$$a(D_e; e - \tilde{e}, \omega_h) + \lambda_e(e - \tilde{e}, \omega_h) = 0, \quad \forall\, \omega_h \in \mathcal{V}_h, \tag{14}$$

$$a(D_p; p - \tilde{p}, \omega_h) + \lambda_p(p - \tilde{p}, \omega_h) = 0, \quad \forall\, \omega_h \in \mathcal{V}_h, \tag{15}$$

$$a(T - \tilde{T}, \omega_h) + \lambda_T(T - \tilde{T}, \omega_h) = 0, \quad \forall\, \omega_h \in \mathcal{V}_h, \tag{16}$$

where $\lambda_s (s = e, p, T)$ are positive constants. It is well known that for $\{\psi, e, p, T\} \in \mathcal{U}$, we have

$$\|\psi - \tilde{\psi}\|_1 \le Ch\|\psi\|_2, \tag{17}$$

$$\|s - \tilde{s}\|_1 + \left\|\frac{\partial(s - \tilde{s})}{\partial t}\right\|_1 \le Ch\Big(\|s\|_2 + \left\|\frac{\partial s}{\partial t}\right\|_2\Big), \quad s = e,\ p,\ T. \tag{18}$$

From (8) and (13), we get the error estimate equation of the electric potential

$$a(\theta_m, \chi_h) = \alpha(p_{h,m} - p_m + e_m - e_{h,m}, \chi_h), \quad \forall\, \chi_h \in \mathcal{V}_h. \tag{19}$$

We choose $\chi_h = I_h^* \theta_m$ as the test function in (19) and obtain

$$\|\theta_m\|_1 \le C\{\|\xi_{e,m}\| + \|\xi_{p,m}\| + h\}. \tag{20}$$

For e, p and T, with the help of the elliptic projections and some other estimate technique, under some suitable assumptions we can get

$$\begin{aligned} &\sup_{1\le n\le N}\{\|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_T^n\|^2\} + C_0\sum_{n=1}^{N}\big(\|\xi_e^n\|_1^2 + \|\xi_p^n\|_1^2 + \|\xi_T^n\|_1^2\big)\Delta t \\ &\le C\big(h^2 + (\Delta t)^2 + (\Delta \bar{t}^0)^3 + (\Delta \bar{t})^4\big). \end{aligned} \tag{21}$$

By (17), (18), (20), (21) and the triangle inequality, we conclude the theorem.

Theorem 1 Let $\{e, p, T, \psi\}$ be the solution of (1)-(5) and $\{e, p, T, \psi\} \in \mathcal{U}$, $\{e_h^n, p_h^n, T_h^n, \psi_{h,m}\}$ be the solution of the fully-discrete implicit Euler characteristic finite volume element scheme (8)-(12), respectively. When $(h, \Delta t)$ is small enough and satisfies $h = O(\Delta t)$, $\Delta \bar{t}^0 = O((\Delta t)^{2/3})$ and $\Delta \bar{t} = O((\Delta t)^{1/2})$, we have a prior estimate in the L^2-norm as

$$\begin{aligned} &\sup_{1\le n\le N}\{\|e^n - e_h^n\| + \|p^n - p_h^n\| + \|T^n - T_h^n\|\} + \sup_{1\le m\le K}\|\psi_m - \psi_{h,m}\| \\ &\le C\big(h + \Delta t + (\Delta \bar{t}^0)^{3/2} + (\Delta \bar{t})^2\big). \end{aligned} \tag{22}$$

4 Numerical experiments

We consider the following system of coupled partial differential equations

$$\begin{cases} -\dfrac{\partial^2 \psi}{\partial x^2} = \dfrac{\partial u}{\partial x} = -e, \quad x \in \Omega = [0,2], \quad t > 0, \\ \dfrac{\partial e}{\partial t} = \epsilon \dfrac{\partial^2 e}{\partial x^2} + u\dfrac{\partial e}{\partial x} + f(x,t), \quad x \in \Omega = [0,2], \quad t > 0, \end{cases} \tag{23}$$

with exact solutions

$$\begin{aligned} &\psi = \mathrm{e}^{t^2}\mathrm{e}^{-37x^2+45x-18}, \quad u = -(-74x+45)\mathrm{e}^{t^2}\mathrm{e}^{-37x^2+45x-18}, \\ &e(x,t) = \left[-74+(-74x+45)^2\right]\mathrm{e}^{t^2}\mathrm{e}^{-37x^2+45x-18}, \end{aligned} \tag{24}$$

where $f(x,t)$ is decided by (24). Let the space-step $h = 0.025$ and the time-step $\Delta t = 0.05$. We use the characteristic finite volume element scheme to solve system (23) and obtain the discrete solution ψ_h and e_h. The error estimates in the L^2-norm of ψ and e are shown in Table 1 and Table 2.

Table 1: Error estimate in the L^2-norm when $\epsilon = 0.01$

L^2-norm	$t = 0.1$	$t = 0.3$	$t = 0.5$	$t = 0.7$
$\|\psi - \psi_h\|$	0.000190	0.000527	0.001001	0.001814
$\|e - e_h\|$	0.002768	0.007080	0.010890	0.017622

Table 2: Error estimate in the L^2-norm when $\epsilon = 0.0001$

L^2-norm	$t = 0.1$	$t = 0.3$	$t = 0.5$	$t = 0.7$
$\|\psi - \psi_h\|$	0.000516	0.001184	0.002232	0.003646
$\|e - e_h\|$	0.003120	0.008211	0.014636	0.026958

From Table 1 and Table 2, we can see that the proposed method is useful and effective even when ϵ is very small.

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一维半导体器件数值模拟的沿特征线的有限体积元方法

龙晓瀚[1], 陈传军[2]

(1- 鲁东大学数学与信息学院，烟台 264025; 2- 烟台大学数学与信息科学学院，烟台 264005)

摘 要: 利用有限体积元方法结合特征线方法来处理一维热传导型半导体器件数值问题。提出并研究了一类全离散隐欧拉特征有限体积元格式。对电子位势和其他未知变量采用不同的时间步长处理，构造了该格式的计算程序，通过理论分析得到了一阶精度 L^2-模误差估计结果。最后给出数值实验验证理论结果。

关键词: 半导体器件；特征线方法；有限体积元方法；误差估计